

The mechanism of O₂ activation and methanol production by (di(2-pyridyl)methanesulfonate)Pt^{II}Me(OH_n)⁽²⁻ⁿ⁾⁻ complex from theory with validation from experiment

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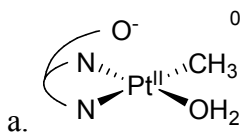
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Supporting Information:

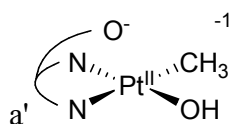
This material includes atomic coordinates of all intermediates and TS shown in this study. Intermediates and TS not given in the main text are also provided here. Eight energies are listed in the following format.

LACVP** in gas phase (Hartree)	LACVP** in water (Hartree)	LACV3P**++ in gas phase (Hartree)	ZPE (kcal/mol)	H correction (kcal/mol)	S _{vib} (cal/mol K)	S _{total} (cal/mol K)	G (kcal/mol)
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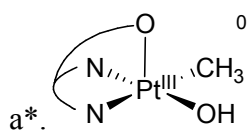
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Pt1	-0.5560704790	0.2754116962	-0.1291190682					
C2	-0.2079370162	-4.5076420480	-0.5336443601					
C3	-1.3087027744	-3.9235933614	0.0839374736					
C4	-1.4434789870	-2.5318615941	0.1310790434					
N5	-0.4866269139	-1.7324182748	-0.4158014602					
C6	0.5646563351	-2.3040705122	-1.0531459805					
C7	0.7394774511	-3.6771896613	-1.1299425030					
H8	-0.0989978535	-5.5882170199	-0.5558458250					
H9	-2.0728466226	-4.5408961026	0.5442451428					
C10	-2.6667491690	-1.9613617693	0.8087869524					
H11	1.2802782915	-1.6240484624	-1.4944938717					
H12	1.6095019531	-4.0733844058	-1.6430871377					
C13	-5.4902885038	0.0973496705	-0.6612186940					
C14	-4.7692783802	1.1646788596	-1.1990511106					
C15	-3.3884700671	1.1703863945	-1.0535614661					
N16	-2.7206028556	0.1937436715	-0.4045341846					
C17	-3.4064756233	-0.8489886026	0.1058348040					
C18	-4.7994385379	-0.9195988381	-0.0084734581					
H19	-6.5718150233	0.0540624687	-0.7547914376					
H20	-5.2597236319	1.9765678733	-1.7263512412					

H21	-2.7842944534	1.9709727065	-1.4696433822
H22	-5.3297080488	-1.7674350980	0.4133286863
H23	-3.3737921894	-2.7891227155	0.8925971084
S24	-2.3985458727	-1.6250023051	2.6445710906
O25	-1.2603417486	-0.6732046647	2.8124408385
O26	-3.7022326326	-1.0674774522	3.0872244073
O27	-2.0907323473	-2.9763773423	3.1812572840
C28	1.4835666830	0.3680093392	0.1659394349
H29	1.8687493828	-0.5329108717	0.6563421202
H30	2.0059689798	0.4872618151	-0.7942668950
H31	1.7354312089	1.2300717641	0.7946871761
O32	-0.5786875884	2.3295103583	0.4418864751
O36	-0.0280836102	1.8226883676	2.9503245140
H37	-0.4651607175	0.9449122430	2.9784020744
H38	-0.3371725662	2.2648195832	1.4243329348
H39	-1.4559416127	2.7464227237	0.4152279451
H40	0.9142904873	1.6434863457	3.0922587697



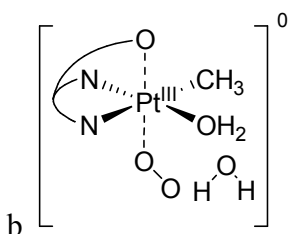
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Pt1	-0.5125142790	0.2232364347	-0.4628450799					
C2	-0.3729001415	-4.6114053952	-0.1190237011					
C3	-1.3854596750	-3.8850526534	0.4976863692					
C4	-1.4468473633	-2.4929696209	0.3633480637					
N5	-0.5082731248	-1.8281418271	-0.3613697389					
C6	0.4566081222	-2.5449464264	-0.9917627635					
C7	0.5605666359	-3.9231681389	-0.8928554079					
H8	-0.3193469685	-5.6902408994	-0.0060998071					
H9	-2.1371617977	-4.3886616637	1.0961430435					
C10	-2.5772174804	-1.7663811169	1.0562782369					
H11	1.1600076711	-1.9727940889	-1.5812431686					
H12	1.3620995496	-4.4356503543	-1.4148861263					
C13	-5.4737463988	0.2378618580	-0.3540832477					
C14	-4.7824218584	1.1718321214	-1.1266806529					
C15	-3.3965223844	1.1074157456	-1.1541516951					
N16	-2.6929575640	0.1870602525	-0.4610448887					
C17	-3.3515756358	-0.7287306626	0.2780492351					
C18	-4.7500734158	-0.7221659397	0.3479284295					
H19	-6.5587633774	0.2542231423	-0.3039036671					
H20	-5.2987097568	1.9343688025	-1.7010930015					
H21	-2.8092590450	1.8075437781	-1.7388136601					
H22	-5.2589078452	-1.4637275324	0.9547256404					
H23	-3.2989647060	-2.5380248638	1.3295361588					
S24	-2.1214661697	-1.1764005939	2.7860430405					

O25	-1.1277129259	-0.0721322572	2.6955521040
O26	-3.4310830401	-0.7372451057	3.3398660160
O27	-1.5709632767	-2.4033293698	3.4218425408
C28	1.5458869858	0.3397539318	-0.3919928128
H29	1.9716977547	0.5323579144	-1.3884048600
H30	1.8152482572	1.1705406325	0.2683005517
H31	2.0153481108	-0.5704163682	0.0009854745
O32	-0.5015330079	2.2735627498	-0.4963601053
O33	0.2427208637	2.4075157619	2.1045841835
H34	0.0619312585	2.4528380482	1.1333765548
H35	-0.1831733878	1.5663083808	2.3346063169
H39	-1.3965323375	2.5680679132	-0.2749606696



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Pt1	-0.5690412874	0.1641117755	-0.4123424522					
C2	-0.4355696275	-4.6935597327	-0.1038397445					
C3	-1.4810737746	-3.9681821657	0.4626728904					
C4	-1.5233859513	-2.5798580996	0.3237320647					
N5	-0.5577391304	-1.9278608576	-0.3732957237					
C6	0.4473391106	-2.6313571397	-0.9376505103					
C7	0.5465344886	-4.0104097278	-0.8188168556					
H8	-0.3876450348	-5.7718721954	0.0174726642					
H9	-2.2607050520	-4.4682555681	1.0278042112					
C10	-2.6076686597	-1.8024411428	1.0365060764					
H11	1.1871097862	-2.0570497855	-1.4819181745					
H12	1.3861504262	-4.5249747103	-1.2743754544					
C13	-5.5661389254	0.1928286971	-0.2592882746					
C14	-4.8979675925	1.1510647235	-1.0215614299					
C15	-3.5141420979	1.0709344201	-1.1214741795					
N16	-2.8025061748	0.1126351523	-0.5003887512					
C17	-3.4364854592	-0.8102804423	0.2508682141					
C18	-4.8269143111	-0.8006133797	0.3816585864					
H19	-6.6469981895	0.2227677413	-0.1558853170					
H20	-5.4281620862	1.9514450656	-1.5275987434					
H21	-2.9424611409	1.7931442300	-1.6958397320					
H22	-5.3167897609	-1.5524979829	0.9921000095					
H23	-3.2890897484	-2.5255571624	1.4899317411					
S24	-1.8789565195	-0.9566006154	2.5298487463					
O25	-0.8701802501	0.0337082260	1.9496105767					
O26	-3.0045440813	-0.2742076162	3.2020647965					
O27	-1.2141797143	-2.0210730559	3.3130695063					
C28	1.4688605712	0.2873087708	-0.0649210366					
H29	1.9935358987	0.5368394046	-0.9934156484					

H30	1.6035962331	1.0791691808	0.6754042839
H31	1.8443318522	-0.6560528982	0.3409293807
O32	-0.5697612608	2.1961779549	-0.3702937629
O33	0.3046332751	2.5779200964	2.2906810872
H34	0.0869042664	2.5812574012	1.3333420363
H35	-0.0673567236	1.7219391011	2.5597761181
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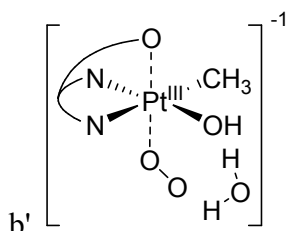
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triplet

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Pt1	-0.3494743800	0.0064291600	0.2493616000
C2	-1.2687688400	-4.6108784100	-0.8070465700
C3	-2.2014444700	-3.8409670600	-0.1168300300
C4	-1.9298966000	-2.5014699400	0.1646505700
N5	-0.7502267800	-1.9490377200	-0.2158600300
C6	0.1519439900	-2.6834576200	-0.9012056300
C7	-0.0753549000	-4.0164709100	-1.2140132600
H8	-1.4775837900	-5.6534323000	-1.0302235700
H9	-3.1472823200	-4.2649795700	0.2004570300
C10	-2.9707819000	-1.6584464100	0.8619046200
H11	1.0583690100	-2.1757735700	-1.2047272400
H12	0.6773081900	-4.5674190000	-1.7678555900
C13	-5.1634491800	0.8853634900	-0.9069649400
C14	-4.1903116800	1.7932553700	-1.3234170200
C15	-2.8594924900	1.5334526000	-1.0124590100
N16	-2.4792505800	0.4420239400	-0.3256427100
C17	-3.4147032600	-0.4384554300	0.0861198000
C18	-4.7685094700	-0.2425588700	-0.1913397000
H19	-6.2122417200	1.0490845000	-1.1371221000
H20	-4.4481918900	2.6865769500	-1.8830286500
H21	-2.0690030300	2.2062579600	-1.3174664100
H22	-5.4966825700	-0.9716726900	0.1493901700
H23	-3.8470743400	-2.2876820200	1.0245287700
S24	-2.4918934200	-1.2333699400	2.6103069100
O25	-3.6795715700	-0.5335714700	3.1569562700
O26	-2.1891236800	-2.5433373900	3.2369737100
O27	-1.2836685300	-0.3358546700	2.5247581000
C28	1.5413775500	-0.4695597900	0.9356115900

H29	2.2690830100	-0.3330744800	0.1304992800
H30	1.7926857400	0.1878099000	1.7751817200
H31	1.5555374300	-1.5050245600	1.2866425200
O32	0.0024110200	2.0394737700	0.7835546600
H33	0.8432055900	2.1540727400	1.2571260300
O34	0.5886285300	0.3648406700	-1.7424382200
O35	-0.1701608900	1.0218524400	-2.5903333200
H36	0.0556382900	2.6320965200	-0.0403499400
O37	0.1475275700	3.3987628400	-1.4097920700
H38	-0.5219075600	4.0640885000	-1.6282384800
H39	0.0575297500	2.6739164500	-2.0761147100



singlet

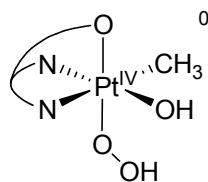
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triplet

-1619.65046	-1619.77092	-1620.07597	173.05	16.19	79.69	161.27	-1016537.2
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Pt1	-0.3993195600	-0.4423072000	-0.0746587400
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C3	-2.3778664600	-4.2511357900	-0.6485155400
C4	-2.0933215900	-2.9178827500	-0.3419635300
N5	-0.8590718900	-2.4094859100	-0.5717485900
C6	0.0916176300	-3.1931219900	-1.1243477900
C7	-0.1313038600	-4.5243963100	-1.4403396500
H8	-1.5988974300	-6.1119115400	-1.4132681000
H9	-3.3737105700	-4.6344359200	-0.4499166100
C10	-3.1700866400	-2.0684260400	0.2833308600
H11	1.0462187800	-2.7255065300	-1.3210804800
H12	0.6783128500	-5.1151008300	-1.8616059800
C13	-5.1729148000	0.8576538000	-1.0447291000
C14	-4.1459652300	1.7622878400	-1.3000630500
C15	-2.8304678400	1.3555453100	-1.0934636800
N16	-2.5148905300	0.1310864700	-0.6281566100
C17	-3.5058786700	-0.7426388100	-0.3606655100
C18	-4.8458381200	-0.4140109600	-0.5751143900
H19	-6.2116060300	1.1390056400	-1.1973976200
H20	-4.3473793900	2.7707073000	-1.6502398300
H21	-2.0002372200	2.0185455200	-1.3109177100
H22	-5.6183273500	-1.1437412900	-0.3542085000
S23	-2.8508882100	-1.8111333800	2.1092492000
O24	-4.0052669000	-1.0064477400	2.5807364100

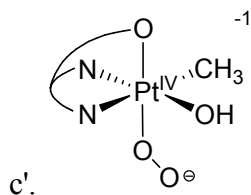
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O26	-1.5465433200	-1.0715409300	2.2127029700
C27	1.4607038200	-0.9865229500	0.6421088800
H28	2.2103292200	-0.7993127800	-0.1339702200
H29	1.7100730900	-0.4051229600	1.5356552700
H30	1.4725554600	-2.0468470800	0.9057483400
O31	-0.0084462900	1.4918055400	0.4323429000
H32	0.9484667500	1.5551535600	0.5830765700
O33	0.5383300200	-0.2673140600	-2.0731529100
O34	-0.2525914100	0.3199447600	-2.9616290200
H35	-0.0131872500	2.4595384800	-1.0100012900
O36	-0.0487669700	2.8515754800	-1.9159938200
H37	-0.0581277900	2.0358655400	-2.4665822000
H38	-4.0817166300	-2.6653676500	0.2931285900



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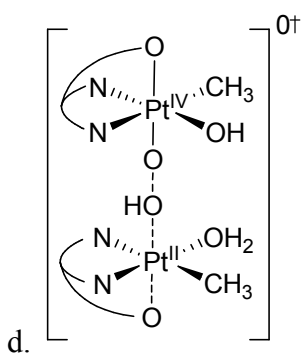
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C2	-1.2837654373	-4.6096248565	-0.8624467548					
C3	-2.2331913147	-3.8426212965	-0.1884240175					
C4	-1.9608006127	-2.5071223705	0.1009111473					
N5	-0.7775170593	-1.9538857783	-0.2568093420					
C6	0.1355031601	-2.6799314328	-0.9304169567					
C7	-0.0840206791	-4.0143693573	-1.2478811277					
H8	-1.4838182813	-5.6539720454	-1.0844404147					
H9	-3.1824910261	-4.2709290132	0.1158224210					
C10	-2.9847825802	-1.6513348502	0.8097053730					
H11	1.0432370877	-2.1647317962	-1.2203285265					
H12	0.6809876276	-4.5664982783	-1.7840831828					
C13	-5.1922014954	0.8941735387	-0.9499183524					
C14	-4.2228753652	1.8188763069	-1.3330650924					
C15	-2.8933673663	1.5678972793	-1.0076814461					
N16	-2.5148988988	0.4656973487	-0.3419713663					
C17	-3.4459391478	-0.4310171591	0.0386593829					
C18	-4.7981741542	-0.2460563795	-0.2495660549					
H19	-6.2395611819	1.0569096508	-1.1877940216					
H20	-4.4813176889	2.7229504122	-1.8753727294					
H21	-2.1059930412	2.2574467461	-1.2816319906					
H22	-5.5261630105	-0.9839906152	0.0714258446					
H23	-3.8547700681	-2.2733917537	1.0312107863					
S24	-2.3934837934	-1.1769415450	2.4988208091					
O25	-3.4919853332	-0.4224810070	3.1315224920					

O26	-1.9896470788	-2.4311975242	3.1626223768
O27	-1.1813854084	-0.2553852352	2.2608140846
C28	1.5147440711	-0.4780182503	1.0216282812
H29	2.2478394154	-0.2902962458	0.2346894930
H30	1.7135865256	0.1418447889	1.8991440196
H31	1.5039402680	-1.5312505513	1.3084987404
O32	-0.0179329341	1.9537668702	0.7869548240
H33	0.8817395094	2.0104454157	1.1459059218
O34	0.5863837531	0.2942542694	-1.4560234972
O35	-0.2547002061	0.9359302911	-2.4125252436
H36	0.0252138401	2.9760818081	-0.5236439665
O37	0.0850984341	3.3928303694	-1.4286566942
H38	-0.6063565849	4.0694720436	-1.4705482562
H39	-0.1048921723	1.9037411532	-2.2117603502



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Pt1	-0.5688264460		-0.0932160336		0.0781738621			
C2	-1.8450694311		-4.7874935677		-0.2956465633			
C3	-2.6271599028		-3.9012864989		0.4435776851			
C4	-2.2572871109		-2.5587088337		0.5279463675			
N5	-1.1368955824		-2.1153686489		-0.0868125644			
C6	-0.3916309638		-2.9601248537		-0.8238748121			
C7	-0.7119037446		-4.3053933350		-0.9492123370			
H8	-2.1213271381		-5.8357203561		-0.3634227539			
H9	-3.5232391910		-4.2407719575		0.9527659458			
C10	-3.1112079372		-1.5760973970		1.2983163280			
H11	0.4682246678		-2.5298015233		-1.3225027814			
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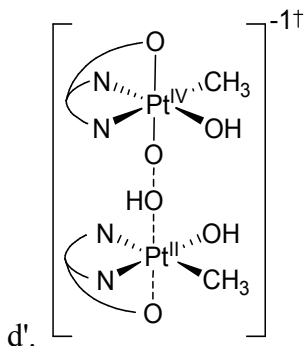
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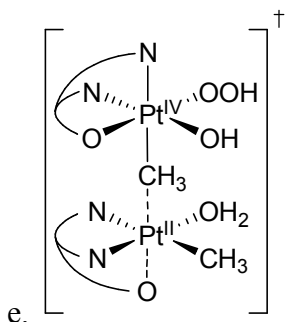
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H74	0.2653644272	2.5231314308	0.4933104924
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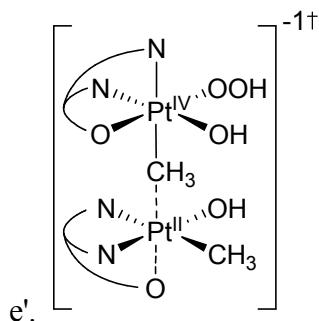
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H40	5.9828023886	-2.1465297862	-3.0924641008
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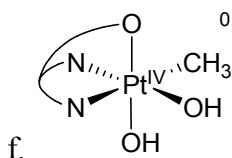
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O26	12.0040283769	-1.1223552809	16.6001130742					
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C28	16.8995289658	-4.2742486494	16.0711104446					
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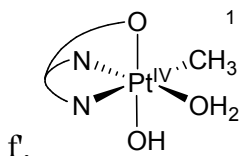
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C18	13.0159725262	-0.9462940999	19.7527343920					
H19	11.8311569593	-1.4411635755	21.4838571472					
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H21	14.5231294474	-4.4434973008	19.9498593855					
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H23	13.9994222159	0.4746300344	17.8967265546					
S24	13.3081019071	-0.9481152903	16.1755454527					
O25	13.6561921217	-2.3462009664	15.7648907797					
O26	11.9133827262	-0.8127003125	16.6650005276					
O27	13.7115841159	0.0627630282	15.1645884579					
C28	17.0524073626	-4.2449425111	15.9438117893					
H29	17.1724994970	-3.5296314592	15.1217768706					
H30	18.0477373734	-4.5622775001	16.2794011292					
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O32	15.2002945428	-5.2742352822	17.8905681347					
H33	15.6825646519	-5.9171276998	17.3499145903					
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C35	16.5043154339	-6.4770870166	24.0273073626					
C36	17.7380862379	-6.9843911838	23.6277409272					

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N38	18.1120261217	-5.0823849560	22.2287523551
C39	16.9143745161	-4.5890919284	22.6143721810
C40	16.0874939601	-5.2523526258	23.5100592039
H41	15.8843641544	-7.0279028526	24.7289612379
H42	18.0974664816	-7.9339802931	24.0115926426
C43	19.8888606719	-6.8299601053	22.3563533788
H44	16.6567245854	-3.6206512034	22.2047659670
H45	15.1388605495	-4.8074729577	23.7928712306
C46	23.1250233448	-6.2209677164	24.2616947987
C47	23.1692886863	-4.8285765621	24.1994440674
C48	22.1396515772	-4.1600152208	23.5358898451
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C51	22.0581797673	-6.8918322500	23.6607018900
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H53	23.9795007001	-4.2656876960	24.6544503374
H54	22.1206099579	-3.0767189744	23.4411250393
H55	21.9917814049	-7.9755135095	23.6903382398
H56	19.8988461605	-7.8849606579	22.6427325208
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O60	18.8513870274	-7.5102949228	19.9942552823
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O65	20.4058195785	-2.5977618166	19.8791486580
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O67	18.4715222546	-2.2318078346	21.7357621812
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H74	12.9536479302	-3.9321290652	16.4571691747
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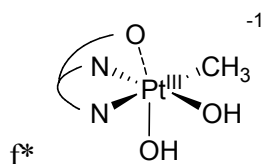
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C3	-1.4784702691	5.4191145507	9.4913454497
C4	-1.2949676648	4.1609285700	8.9228317115
N5	-2.1068851066	3.7383695169	7.9240364669
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C7	-3.3068278616	5.8011975489	7.9755069085
H8	-2.6476939390	7.2298652549	9.4560646775
H9	-0.8277503412	5.7403304480	10.2979806649
C10	-0.1920807949	3.2424187262	9.4042309712
H11	-3.6720583331	4.1393581904	6.6313113654
H12	-4.1064279210	6.4123439436	7.5696250970
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C14	2.6479474989	2.1769929657	6.4029282339
C15	1.2785810676	1.9685565251	6.2565565050
N16	0.4098812354	2.3154787295	7.2195168858
C17	0.8480103755	2.8817946504	8.3607252279
C18	2.2050459768	3.1145856222	8.5762808528
H19	4.1797287173	2.9253593536	7.7286404523
H20	3.3240491322	1.8856874819	5.6051597157
H21	0.8515766884	1.5199196748	5.3621182274
H22	2.5385279622	3.5680033285	9.5041958086
H23	0.3075541579	3.7200281675	10.2499067807
S24	-0.9114628641	1.7178285562	10.1828108043
O25	0.2154893112	0.9468455574	10.7352640452
O26	-1.9317809140	2.1840678309	11.1386225021
O27	-1.5645659173	0.9229792810	9.0200909057
C28	-3.8078936427	1.3792463732	7.1444546912
H29	-4.2496760320	1.7798025709	6.2310141982
H30	-3.8795948126	0.2926685564	7.1698581488
H31	-4.2617771812	1.8228980731	8.0318034695
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H33	-0.8082257263	-0.4028778534	6.9661123440
O34	-2.0308568127	2.6261027853	5.2948448661
O35	-0.6230100480	0.6642116942	3.8863689624
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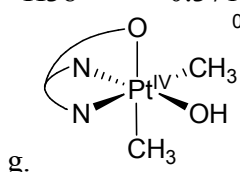
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C3	-1.1934989818	5.5487246208	9.1230091735					
C4	-1.1462529115	4.2256812890	8.6925295076					
N5	-2.1009051503	3.7322348372	7.8668657490					

C6	-3.0974829330	4.5283136541	7.4336620302
C7	-3.1901930759	5.8593215178	7.8226403314
H8	-2.2766809283	7.4093891070	9.0209137633
H9	-0.4277876001	5.9190140097	9.7969579549
C10	-0.0337173364	3.3095506663	9.1468186562
H11	-3.8229448292	4.0812937286	6.7646155557
H12	-4.0111992266	6.4651732650	7.4534736777
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C15	1.0044997738	1.5158405469	6.0843847613
N16	0.2560574239	2.0642345061	7.0530414831
C17	0.8502269751	2.7528962461	8.0484315959
C18	2.2326487867	2.9229717878	8.0937051912
H19	4.0938015174	2.4862114065	7.0955029117
H20	2.9616975294	1.1950893129	5.2557411048
H21	0.4769087333	0.9437713310	5.3288529644
H22	2.6853536295	3.4762019350	8.9105206283
H23	0.5895874572	3.8497197661	9.8633317893
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O25	0.3982021143	1.1470882774	10.6953954070
O26	-1.6347668055	2.5539265537	11.1619834115
O27	-1.5381897364	1.0478834902	9.1716558766
C28	-3.9912873603	1.3484172056	7.7435602261
H29	-4.6051816544	1.8147116062	6.9714385989
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H31	-4.1793195418	1.7821634366	8.7260022816
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H33	-1.7244349873	-0.7193433714	7.4748336899
O34	-2.6420601695	2.1336141630	5.3724448067
O38	-1.1611415939	3.0606856647	3.5557402621
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H40	-1.9777650080	2.4890673047	4.6514287794
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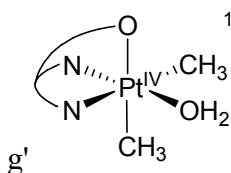
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C7	-3.8571011072	5.1213980157	7.4721859704
H8	-3.5691347599	6.9278503970	8.6266582939
H9	-1.4224954669	6.1195906996	9.6074942935
C10	-0.1962410432	3.7639735349	9.2140963255
H11	-3.7994959863	3.2040653145	6.4811074544
H12	-4.7843737041	5.4264904534	6.9975562064
C13	3.1516171888	3.2344524280	7.5096938606
C14	2.7966158779	2.2780544427	6.5591550735
C15	1.4773671975	1.8394471574	6.5121022250
N16	0.5373455051	2.2997366341	7.3601421420
C17	0.8630847266	3.2384026526	8.2717454679
C18	2.1706003188	3.7235463533	8.3696504627
H19	4.1725094434	3.6001569894	7.5786110078
H20	3.5216306744	1.8746184236	5.8587239572
H21	1.1401656346	1.1125430857	5.7774708632
H22	2.4098185437	4.4759263770	9.1143186264
H23	0.2334773748	4.6262471804	9.7277871266
S24	-0.4888509903	2.6087292444	10.6518882779
O25	0.8774996959	2.3161076426	11.1601857169
O26	-1.3285883400	3.4106079889	11.5815117556
O27	-1.1938324955	1.4045225185	10.1184688691
C28	-3.4532519147	0.7331110147	7.3391352614
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H30	-3.4428842871	-0.3346383555	7.5925385017
H31	-4.0541362825	1.2556784982	8.0909796919
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H33	-1.6403074788	-0.9800439396	6.9420318853
O34	-1.6633296534	2.1233442058	5.1047369700
H71	-1.0657697515	2.8867156869	5.1350799598
H36	-0.7266263324	0.8369816368	4.5190923988
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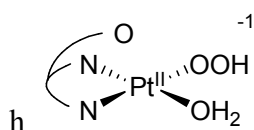
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C4	-1.8712794769	-2.5866162028	0.2219903390					
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C6	0.2736516463	-2.6205987933	-0.7130975406					
C7	0.2122876732	-3.9917828940	-0.9212392006					
H8	-1.0181204809	-5.7536384294	-0.6763018103					
H9	-2.8963174077	-4.4671132843	0.3491502029					

C10	-3.0035954768	-1.8229236721	0.8695715793
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H12	1.0585370681	-4.4986306054	-1.3735566197
C13	-5.4782320126	0.4906570830	-0.8495432111
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C17	-3.5896524302	-0.6774876661	0.0737208819
C18	-4.9628187192	-0.6093615427	-0.1646604433
H19	-6.5454574114	0.5639407033	-1.0400582022
H20	-4.9681560087	2.3726283506	-1.8007646028
H21	-2.5288423385	2.1181392902	-1.2896713373
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H23	-3.8040494590	-2.5330782994	1.0866801301
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O25	-3.6939228264	-0.5549204884	3.1198764422
O26	-2.0955398342	-2.4722649253	3.2935538706
O27	-1.3408029015	-0.3002477448	2.3490508774
C28	1.3577982177	0.0160307090	0.8982427656
H29	2.0700042704	0.4396437439	0.1860872669
H30	1.3566490367	0.5940483128	1.8249133169
H31	1.6139423439	-1.0252758627	1.1083326096
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H37	1.0669788383	0.1252190884	-1.8730252372
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O38	-0.2073415175	2.1026128063	3.2868068946
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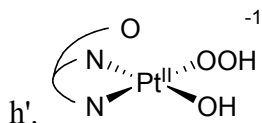
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C7	-0.0844981413	-3.5878067540	-1.7882762586					
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C13	-5.8393451305	-0.5725438950	0.3874470183
C14	-5.3937011407	0.6022029544	-0.2200064478
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S24	-1.5473025171	-1.3729810768	2.8376647965
O25	-2.5587817990	-0.7902002769	3.7462468497
O26	-0.7582295124	-2.5012067661	3.3810780430
O27	-0.6360121215	-0.3024274413	2.2331579992
C28	1.2347986374	0.2986072151	-0.1378102054
H29	1.5121772202	1.0635764360	-0.8662113023
H30	1.5959389673	0.5610468002	0.8570731569
H31	1.6193047929	-0.6771425651	-0.4357805792
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O38	1.0701879810	2.1706513109	2.7322428502
H39	0.0016968783	2.2708558627	1.4489095086
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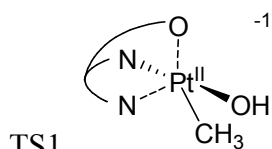
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H11	-2.7895644748	3.0719951758	9.5318372824
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C15	-2.6711392853	2.4510431892	3.9740706953
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C17	-1.1503483103	3.9981028632	4.8638316961
C18	-0.8881210655	4.4741110625	3.5743176620
H19	-1.2965745362	4.2699744072	1.4695141823
H20	-2.9446700870	2.3914435650	1.8554725916
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H23	-0.0498305756	5.5887619101	5.6672589385
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O27	1.0673725181	2.3888509544	6.7438883817
O32	-2.9847097926	0.4232161833	5.9146299473
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O33	0.3119560528	0.3124358546	8.4105242263
H34	-1.2627819350	0.6095450562	8.6335582177
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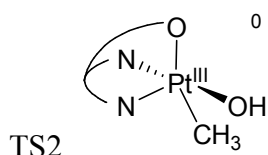
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N5	-1.8765155692	3.9087283018	7.8549146946					
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H8	-0.9679992499	7.1008882922	9.8438416972					
H9	0.0368766050	6.6609547320	7.6044144850					
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H12	-2.5981440591	5.4158347727	10.7819713045					
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C14	-2.5647151211	2.9807496615	2.7141236611					
C15	-2.7063596963	2.4828585282	3.9999434961					

N16	-2.0208861525	2.9833535558	5.0542203484
C17	-1.1581377072	4.0097319047	4.8623053513
C18	-0.9811137058	4.5559612897	3.5865222733
H19	-1.5490103713	4.4624468490	1.5088846665
H20	-3.1376097033	2.5400984991	1.9045186273
H21	-3.3635792029	1.6504748475	4.2208145535
H22	-0.2821813711	5.3749129836	3.4545858871
H23	0.0765296677	5.4967841955	5.6764764593
S24	1.2745770627	3.5666464498	6.1982103706
O25	1.9011183320	3.6969622535	4.8566927423
O26	1.9886595787	4.2892216949	7.2829916943
O27	0.9490369945	2.1531454943	6.5435801803
O32	-2.6225041322	0.3713620691	5.9531962079
O34	-2.5375252753	1.2357096161	8.7260355661
H41	-2.8745288614	0.3581684485	8.4762751102
O31	-2.3859080043	-0.7803957740	6.8313225731
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H35	0.2741880136	0.8117336333	7.6673129893



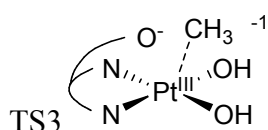
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N5	-0.7591854131	-1.9694422873	-0.1877527756					
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C7	-0.0907559061	-4.1930257864	-0.8634430891					
H8	-1.5251028937	-5.7727947517	-0.5016085614					
H9	-3.1361200773	-4.2231887428	0.5986484939					
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H12	0.6766749844	-4.8157435874	-1.3121703944					
C13	-5.9104549774	0.5425674109	0.4538600297					
C14	-5.3046823414	1.5359158488	-0.3162040216					
C15	-3.9593129867	1.3798502717	-0.6479143180					
N16	-3.2251942239	0.3365807185	-0.2474833029					
C17	-3.7933840101	-0.5988173214	0.5206270655					
C18	-5.1451312313	-0.5420417324	0.8829131532					
H19	-6.9584198953	0.6179613226	0.7309382980					
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H23	-3.5445479020	-2.3791442523	1.6438811651
S24	-2.0161264779	-0.8664924547	2.5682415882
O25	-3.0761480249	-0.4875018348	3.5339954093
O26	-1.0585242195	-1.8816517851	3.0756229131
O27	-1.3362772671	0.3394721544	1.9661867759
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H29	0.5583615477	-0.7641579889	-2.6636429530
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O34	-1.5632260774	3.1181553983	1.5941643785
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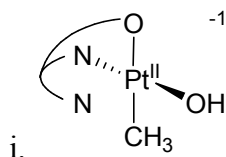
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C3	-0.9476924685	-3.8440057985	0.5456391442					
C4	-1.3300784545	-2.5223814429	0.2946366538					
N5	-0.5286213000	-1.6943179351	-0.4317551618					
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C7	1.0380038404	-3.5014416532	-0.7374345770					
H8	0.5540780592	-5.3623306767	0.2566424729					
H9	-1.6002124074	-4.4740890140	1.1405745914					
C10	-2.6562972840	-2.0722980415	0.8581478737					
H11	1.2128885720	-1.5313725290	-1.5543273809					
H12	1.9745077528	-3.8314172013	-1.1750766143					
C13	-5.7030902998	-0.8062096303	-1.0089729580					
C14	-5.1474055658	0.2987788095	-1.6568113382					
C15	-3.7995289979	0.5719220607	-1.4686986980					
N16	-3.0205505451	-0.1914620518	-0.6737952404					
C17	-3.5417846986	-1.2628103751	-0.0455283139					
C18	-4.8915053957	-1.5937499463	-0.1967766236					
H19	-6.7536802979	-1.0522169721	-1.1371380557					
H20	-5.7416559162	0.9402975007	-2.2994403109					
H21	-3.3174650532	1.4141776775	-1.9521976473					
H22	-5.2915827042	-2.4595406117	0.3206799676					
H23	-3.2028093815	-2.9791077178	1.1238146719					
S24	-2.5091878725	-1.2517305477	2.5391163405					

O25	-1.9614483872	0.1169923693	2.2885540867
O26	-3.9072082736	-1.2327572887	3.0369840900
O27	-1.5884408771	-2.1297754106	3.3018373582
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H29	1.7480949367	0.3889557612	-0.4574243958
H30	1.1100353179	0.3873164225	-2.1459727461
H31	1.1175241219	1.8991316913	-1.1911286079
O32	-1.0602731823	2.2993152583	-0.1264190330
O33	-0.4662029360	2.3704651027	2.5810104454
H34	0.4905899208	2.2314976310	2.5159044955
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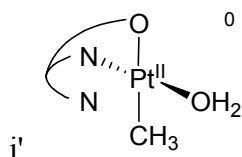
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C4	-1.5423769982	4.0988607570	9.0164880816					
N5	-2.0090143006	3.7356191824	7.7995625708					
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C7	-3.6612693341	5.4815137092	7.9045254995					
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H9	-1.7394669559	5.4283348219	10.6907342758					
C10	-0.4102175746	3.3642279618	9.6746037803					
H11	-3.3647644611	4.0624313266	6.2889164840					
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C14	3.0183334928	2.0945096283	7.4843854518					
C15	1.7373958823	1.9709125160	6.9700318450					
N16	0.6345617571	2.3801014636	7.6422933939					
C17	0.7805078461	2.9436875844	8.8641474836					
C18	2.0522402225	3.1038524385	9.4263089084					
H19	4.1706200577	2.7894824349	9.1805910469					
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H21	1.5346847625	1.5148916029	6.0094869618					
H22	2.1397259346	3.5572559255	10.4085168597					
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O27	-0.3461804081	0.6865141059	10.2248121831					
C28	-2.3164719052	0.0390680855	7.7080130669					
H29	-3.1008657490	0.4442546363	8.3370894106					

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H31	-1.4992386494	-0.4244744652	8.2474584239
O32	-0.3709804737	0.6999725214	5.5184571134
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O34	-2.9763235437	2.0768306411	5.6466743226
H71	-3.6391029363	1.7437783988	6.2693171540
O36	-2.5527233901	-0.1562939663	4.2064886863
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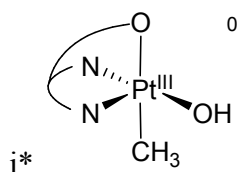
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O25	2.0275974545	3.9688681055	8.1174152601					
O26	1.2590264317	1.6707041917	8.6929383821					
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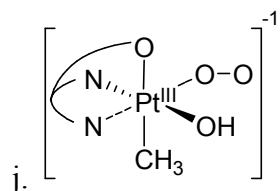


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H21	-4.0909729099	3.7996505870	6.7068172676					
H22	-0.8868924180	6.2331864228	9.4842962836					
H23	0.4480962810	4.5074392181	9.5132038295					
S24	1.0397900530	3.2522513135	7.6834734865					
O25	1.5829801519	4.5532828577	7.2289202755					
O26	2.0420695320	2.3234863402	8.2555588175					
O27	0.2277473781	2.6001152020	6.5762049097					
C28	-3.7625546507	1.2084892115	7.2421188066					
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H30	-3.7190497760	0.1311952763	7.4406679670					
H31	-4.2373913183	1.7035151809	8.0964102574					
O32	-1.2941487908	0.0414427952	6.1209053764					
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O34	0.6299652976	-0.2647076824	7.8243128826					
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C7	0.2993480660	-4.0133144121	-1.2767082293					
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C17	-3.4696080927	-0.9521714893	0.2804208898					
C18	-4.8587455622	-1.0980260612	0.2943011816					
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H23	-3.2303155713	-2.6420557004	1.5382631514					
S24	-1.8224986727	-1.0472787875	2.5201100923					
O25	-0.8149738605	-0.0624292412	1.9557012122					
O26	-2.9422849708	-0.3616941432	3.2033694669					
O27	-1.1646014349	-2.1232094826	3.2951568726					
C28	-0.3470477253	0.3826452798	-2.3658176327					
H29	0.7049919876	0.2441100932	-2.6389436656					
H30	-0.9710712989	-0.3552658074	-2.8777286410					
H31	-0.6620283318	1.3939942169	-2.6370677797					
O32	-0.3168759031	2.1215489884	-0.0780867971					
O33	-2.3589992500	4.0327119658	-0.8808579093					
H34	-1.8649764105	4.8466776261	-1.0647987921					
H35	-2.7285899727	4.1920388203	0.0014034213					
H39	-1.0187662809	2.6368264590	-0.5186584466					



j.

singlet

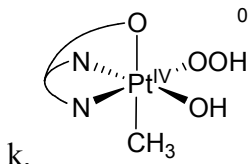
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triplet

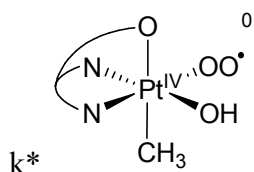
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C2	-1.3621059600	-4.8421264700	-0.1803132300
C3	-2.2983863800	-3.9551827800	0.3451441500
C4	-2.0434340300	-2.5822753700	0.3537688900
N5	-0.8990738500	-2.0896061800	-0.1820012600
C6	0.0078414100	-2.9444708500	-0.6992906300
C7	-0.1807778100	-4.3222801500	-0.7051783200
H8	-1.5478414700	-5.9142083900	-0.1588958200
H9	-3.2205313700	-4.3210046800	0.7815889200
C10	-3.0160167000	-1.6531872200	1.0500247800
H11	0.9170288000	-2.4898752100	-1.0773410100
H12	0.5987505400	-4.9656458800	-1.0975359300
C13	-5.6285745600	0.6367826600	-0.4873632600
C14	-4.7921065300	1.5776965900	-1.0855690400
C15	-3.4131502700	1.3961317800	-0.9956497700
N16	-2.8713566800	0.3595903800	-0.3445705800
C17	-3.6650137400	-0.5470040700	0.2417368100
C18	-5.0582602800	-0.4430046800	0.1841751100
H19	-6.7087679700	0.7364173100	-0.5507666200
H20	-5.1932950700	2.4364858100	-1.6115396600
H21	-2.7193271200	2.1103073500	-1.4345032100
H22	-5.6833817600	-1.1903729500	0.6636189100
H23	-3.8210410700	-2.2639345100	1.4663845500
S24	-2.2216437100	-0.9681900500	2.5900413400
O25	-3.2519150100	-0.0948586100	3.2016870100
O26	-1.8530465000	-2.1638610900	3.3865908600
O27	-0.9948102200	-0.1884581700	2.1581840300
C28	-0.0241372500	0.1043788000	-2.1130976700
H29	-0.2299245800	-0.8575173600	-2.5942019700
H30	-0.6286250000	0.8893460000	-2.5818073500
H31	1.0381101300	0.3357153400	-2.2042529800
O32	-0.0621632500	1.9561988600	0.0500947800
O33	1.8303290300	-0.7037020500	0.0506269600
O34	2.8124110700	0.1577104800	0.2069448000
O35	2.0345055100	1.9384301100	2.0627828100
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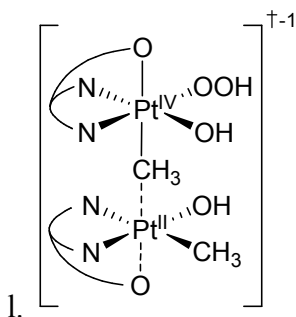
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C3	-3.0385880312	-1.3448931372	3.3737629128					
C4	-2.3718247859	-1.1378375772	2.1670244337					
N5	-1.2062185152	-0.4538837815	2.1366934050					
C6	-0.6781252559	0.0464833940	3.2693403893					
C7	-1.2951298492	-0.1319415042	4.5011795244					
H8	-3.0066393186	-0.9962982105	5.4998902097					
H9	-3.9771399373	-1.8898731533	3.3783009026					
C10	-2.9708903634	-1.5931823376	0.8602518396					
H11	0.2339262787	0.6201556972	3.1565101531					
H12	-0.8423203045	0.2920763283	5.3914602202					
C13	-1.7304754867	-4.4287119268	-1.3440770537					
C14	-0.5044662577	-3.9031817960	-1.7488538904					
C15	-0.1153057665	-2.6610553796	-1.2651150821					
N16	-0.8909134700	-1.9597534597	-0.4153960796					
C17	-2.0934618404	-2.4440348416	-0.0244883840					
C18	-2.5337645104	-3.6859255770	-0.4794784232					
H19	-2.0646128118	-5.3987509032	-1.7010237043					
H20	0.1494053383	-4.4368044639	-2.4310734977					
H21	0.8133535361	-2.1913045390	-1.5659827762					
H22	-3.5007468977	-4.0588605434	-0.1580890169					
H23	-3.8871559916	-2.1474909062	1.0713675312					
S24	-3.5875384424	-0.1053187558	-0.0862056245					
O25	-4.1657860227	-0.6393567766	-1.3372379992					
O26	-4.5356877768	0.5753943686	0.8216315095					
O27	-2.3444832549	0.7360888978	-0.3360330270					
C28	1.5479447121	-0.8915378035	0.9296095228					
H29	2.1846879265	-1.0011072535	0.0499150239					
H30	1.9794730327	-0.1849767743	1.6398222652					
H31	1.3411187096	-1.8537084763	1.4000120570					
O32	0.3446567215	1.7146182935	0.9330790982					
H33	1.2283614290	1.8451984720	0.5496104598					
O34	0.7364978352	0.2869667630	-1.4243930589					
O35	-0.1717600317	0.8434513644	-2.3910479278					
H36	-0.5019935230	2.7255052448	-0.2175757289					
O37	-0.9569189010	3.0722235065	-1.0266624048					
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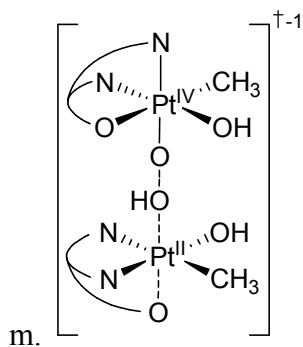


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C3	-0.8276663777	1.6382950099	11.2630095411					
C4	-1.0300119077	2.0581697773	9.9498366646					
N5	-1.7911115645	1.3208496580	9.1086380722					
C6	-2.3642858082	0.1728749522	9.5233471184					
C7	-2.1955654037	-0.2914891283	10.8209893696					
H8	-1.2605429720	0.1158250580	12.7256193946					
H9	-0.2113263004	2.2369274829	11.9255831164					
C10	-0.3814222701	3.3158314374	9.4246314255					
H11	-2.9465589987	-0.3738578434	8.7915865178					
H12	-2.6686040993	-1.2217769472	11.1182263769					
C13	-2.1633472018	6.5792914556	8.6446258535					
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N16	-2.1379715849	3.9393491191	7.7994072111					
C17	-1.3180552106	4.3270571675	8.8076488918					
C18	-1.3150256540	5.6495843028	9.2454828628					
H19	-2.1605736771	7.6138984318	8.9751064116					
H20	-3.6816819155	6.8444935158	7.1147239579					
H21	-3.5818422255	4.4571837694	6.4097656210					
H22	-0.6465807591	5.9423077446	10.0483990784					
H23	0.1485550952	3.7979037552	10.2485731009					
S24	1.0000413020	2.8958038867	8.2408671452					
O25	1.6212555278	4.1853341921	7.8784529345					
O26	1.8607144268	1.9345750455	8.9586575930					
O27	0.3003860328	2.2527005805	7.0455244137					
C28	-4.0270935887	1.6678907550	7.1371071571					
H29	-4.4286052945	2.2644960304	6.3182718143					
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O34	-2.0243982261	2.4581337023	5.1253532297					
O35	0.4243098998	0.5327607169	4.7282797523					
H36	-0.4014834536	0.2995719860	5.2009909108					
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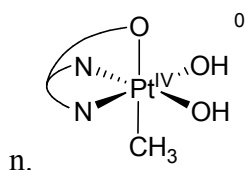
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Pt3	0.7488923763	0.6556324514	0.6459052901					
Pt4	-1.6279301446	-3.2616384672	-0.9118738239					
C5	-2.7840663900	-4.1062374166	3.8645539943					
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C8	4.1304167303	-1.7848506729	-0.4824199534					
C9	-1.1929755546	-3.6971908208	2.1239122619					
C10	2.9449536461	-1.0650874219	-0.4337054897					
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C13	-3.4442302057	-3.8512615587	1.5575985839					
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H17	-3.0350834302	-4.2790377402	4.9075410546					
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H20	4.4405310706	-2.2388099361	-1.4184358211					
H21	-4.8230353863	-4.2340112830	3.1665018565					
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C23	-5.9929512966	-1.2267679645	-1.7115607287					
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C25	-4.8654840038	-0.8256893856	-2.4259460696					
C26	-1.2519531179	-0.0636692826	4.3942539701					
C27	-3.6494295654	-1.4325274517	-2.1494634796					
C28	-0.9182807311	0.1988145106	3.0732764595					
N29	-3.5073610557	-2.4116275097	-1.2249030616					
N30	0.3627455154	0.2254924320	2.6457766637					
C31	-4.5981974610	-2.8053590833	-0.5178786227					
C32	1.3700779391	0.0094317301	3.5241224414					
C33	-5.8474418328	-2.2200632029	-0.7495354854					
C34	1.0912507067	-0.2693057629	4.8645640120					
H35	-6.9643505833	-0.7772975849	-1.8969320474					
H36	-0.4498563497	-0.5248724345	6.3497868364					
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H38	-2.2961266960	-0.0681853936	4.6900792920
H39	-6.7013844243	-2.5578928942	-0.1717387125
H40	1.9132732205	-0.4398019711	5.5518216678
C41	2.8021060003	0.1565491433	3.0797287482
C42	-4.5162148242	-3.9169719746	0.4986617355
H43	3.4345286705	-0.1929629288	3.8980572794
H44	-5.4769483687	-3.9409638462	1.0167675070
S45	3.2711656120	1.9761741385	3.0011989618
S46	-4.5342108646	-5.5939517755	-0.3405934508
O47	2.3823929619	2.5990195620	1.9684890511
O48	-3.2862297660	-5.6979051281	-1.1632795071
O49	4.7027307307	1.9662103061	2.6137271988
O50	-4.5749677529	-6.5606016058	0.7849846511
O51	2.9976481197	2.4726261004	4.3724214017
O52	-5.7633714117	-5.5560238930	-1.1740258606
C53	-1.1014736257	-3.0654340126	-2.8978459773
C54	-0.5017253035	-1.1693465803	-0.2005380955
H55	-1.9566890463	-3.3243650584	-3.5339150925
H56	-1.3808927855	-0.9184742495	0.3747058473
H57	-0.7710023070	-2.0515875611	-3.1569806887
H58	0.2248738498	-1.8770276661	0.1665040659
H59	-0.2808936586	-3.7560125252	-3.1330931273
H60	-0.4165302505	-0.8070200991	-1.2142600911
O61	0.1897125119	-4.0873056881	-0.5126751782
O62	1.1438475231	1.1389653954	-1.2886306817
H63	0.7370951992	-3.9964987844	-1.3066669104
H64	0.2849752291	1.4786753758	-1.5972720862
H65	-2.7540697243	-1.1449733145	-2.6828464780
H66	-1.6746343782	0.4262709106	2.3301290947
H67	2.3256503588	-0.9140613227	-1.3092103679
H68	-0.1821249736	-3.5772269065	1.7503708542
H77	-0.2267136939	3.2835398060	-0.3569028553
O70	1.5394303540	3.7065038808	-0.4938798454
H71	1.6021666705	2.8063005127	-0.9003379063
H72	1.9342018378	3.5623398860	0.3843206066
O76	-0.6999047428	-6.6299389571	-0.5357215572
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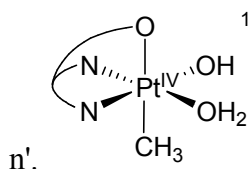
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Pt3	2.7915659876	-0.3612165463	-1.4442932943					
Pt4	-2.3395392719	0.3577977285	0.0636278329					
C5	-3.4803637979	3.9590160292	-3.2727055691					
C6	5.8432112700	-3.9762927357	-0.4067955619					
C7	-2.2427288234	3.9795875760	-2.6323012910					
C8	4.9982924351	-3.4611338331	0.5754989277					
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C10	4.1467602537	-2.4150061670	0.2452045069					
N11	-2.7669788906	1.9280822236	-1.5003958148					
N12	4.1235904400	-1.8891209804	-0.9955580224					
C13	-3.9735650094	1.9058333313	-2.1065975001					
C14	4.9257448664	-2.3837977189	-1.9673084080					
C15	-4.3539946734	2.9089492053	-3.0029460008					
C16	5.8005254434	-3.4335802245	-1.6902235973					
H17	-3.7662478470	4.7468972613	-3.9641110304					
H18	6.5206963175	-4.7955847584	-0.1829167410					
H19	-1.5286387861	4.7802527549	-2.8003819370					
H20	4.9875279588	-3.8587788471	1.5852309498					
H21	-5.3316461283	2.8647731304	-3.4721350424					
H22	6.4347487830	-3.8204301368	-2.4813186232					
C23	-4.7262594720	-2.8607983197	-2.6710671666					
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C25	-3.5430357633	-3.2055908056	-2.0193802220					
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C27	-2.8807416390	-2.2356634306	-1.2802133640					
C28	4.3238483550	1.8279616326	-2.9467577817					
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C31	-4.4669499882	-0.6085891440	-1.8288643880					
C32	5.0207831408	-0.3325163468	-3.5023661811					
C33	-5.1777223474	-1.5472699543	-2.5824290646					
C34	5.9720992370	0.1775356231	-4.3852220235					
H35	-5.2809054786	-3.5953630184	-3.2481851819					
H36	6.8303771899	1.9686559265	-5.2237318453					

H37	-3.1295676107	-4.2076261460	-2.0751156362
H38	5.2947625964	3.4770925595	-3.9124701774
H39	-6.0825334227	-1.2367849620	-3.0947539268
H40	6.6023275159	-0.5053025321	-4.9459145225
C41	4.8135262571	-1.8216407919	-3.3630517580
C42	-4.9655073136	0.8136216384	-1.7741544682
H43	5.5407151587	-2.3332769054	-3.9963079687
H44	-5.7787891791	0.8884583613	-2.4989534565
S45	3.1807558137	-2.3176220043	-4.1278929723
S46	-5.8793457421	1.1909956933	-0.1864369033
O47	2.1135571355	-1.6079007861	-3.3168370732
O48	-4.8908131571	1.1071133451	0.9305304478
O49	3.1179299565	-3.7887298487	-3.9767614536
O50	-6.4083874900	2.5645253926	-0.3992874269
O51	3.2412950552	-1.8206459338	-5.5210554128
O52	-6.9282401189	0.1374850742	-0.1222202567
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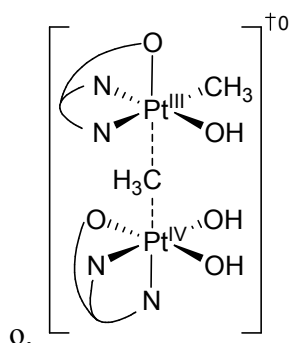
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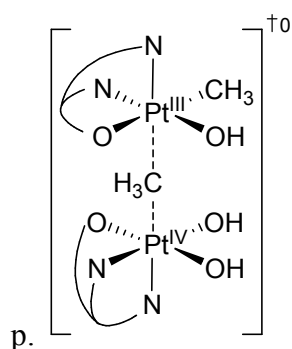
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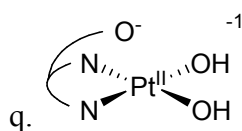
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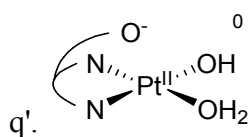
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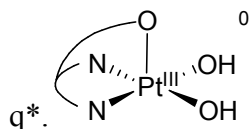
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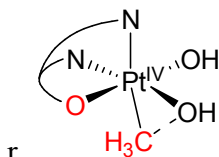
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H11	-3.1653437252	3.1441879663	9.4370573885					
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C18	-1.2209606794	4.5124011135	3.5832532457					
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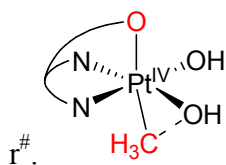


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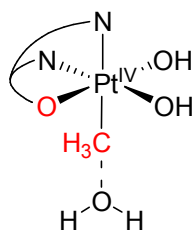
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N5	-1.9282386873	3.7792475716	7.9097807406					
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C10	-0.2579010906	2.8454849805	9.5815552486					
H11	-3.2882906925	4.6573759676	6.6214547895					
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C13	3.5369777697	2.7055734034	9.4214636378					
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H19	4.3816830407	2.4377189189	10.0500186704					
H20	4.7256251185	3.2084359997	7.6750556975					
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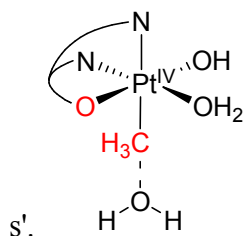


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C17	-1.0003508077	4.6375256896	7.2464096128					
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O27	-0.4899084866	1.4215153239	7.1940477292					
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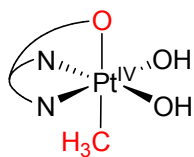
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C10	0.9019541949	-2.2238644910	1.6939244801					
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H37	-2.0933989983	1.2673549368	-1.7186593383					
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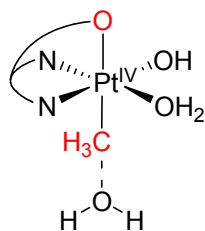
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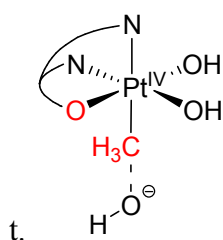
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C7	-0.0248834912	-4.4227144915	-0.4441800491				
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C17	-3.2939101840	-0.3968671164	-0.0152857742				
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H19	-5.9023082774	1.5061397399	-1.0965511612				
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H23	-3.9953222802	-2.2163425173	0.7737265403				
S24	-2.8046655708	-1.2863875743	2.5784638844				
O25	-3.9957801520	-0.4732910518	2.9376771498				
O26	-2.7599352859	-2.6257838418	3.2210654431				
O27	-1.5191848315	-0.5367723180	2.6735997266				
C28	0.3468984466	0.3147707162	-2.5401735236				
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H30	1.1624931134	-0.3873702398	-2.4393847746				
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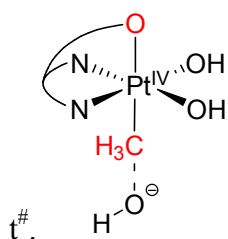
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C6	0.1731848085	-2.9091625095	-0.6999001344					
C7	-0.1528278684	-4.2398879650	-0.9102677275					
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C10	-2.9946443377	-1.4299501511	0.5868865728					
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H23	-3.9717059937	-1.9158134457	0.5978508950					
S24	-2.6552264919	-1.1821806559	2.4184075213					
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H31	-0.4439728914	-0.5531764054	-2.6205928855
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H37	0.3380561123	2.1942872027	1.2338903242
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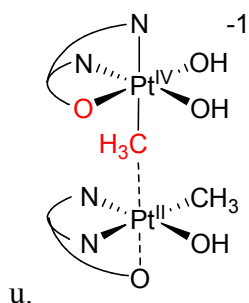
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O43	2.5295867864	-0.6697505418	-7.7097333737
H44	2.4406100811	-1.1865141628	-6.8807451061
H45	2.6901242037	0.2281973326	-7.3508438202
O46	2.1309810573	-1.8187169510	-5.0988649545
H47	2.1173139222	-0.9088413257	-4.6521074598
H48	1.1946147430	-2.0182094164	-5.2486649474
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H49	-3.6669005627	2.7283676503	-0.0372801118
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H12	1.3941514799	-4.7268822287	-0.8849288018					
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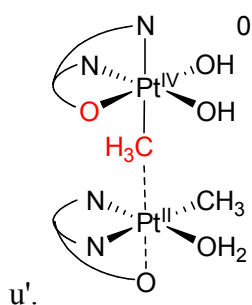
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H20	-4.2698885719	2.2342981917	-2.4847468271
H21	-1.9460591389	1.9588319952	-1.6180793810
H22	-5.3130962206	-1.3806387315	-0.3695399692
H23	-3.7263130592	-2.5588526799	0.7065068517
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O34	1.5886876279	-0.1359992917	0.5686658569
H36	2.3415627617	0.9921823959	-3.7216725134
O37	1.4989622388	0.7060328915	-4.1117237999
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H44	1.3567274333	0.5969973895	-7.4007212700
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O47	2.6087884621	2.3606267572	0.7044199373
H49	2.3423602594	1.4023398036	0.6891562755
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N5	16.8810252979	-2.0144073920	16.5071112885
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C17	14.6788881753	-0.3717495177	18.0240634613
C18	14.0269570246	0.7372779322	18.5741623940
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H20	13.7920857695	-0.4205030877	21.7594883791
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O26	12.3575856949	-0.6342359345	16.0941641880
O27	13.9157480931	-0.9761511822	14.1725379781
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C37	21.5257204103	-5.9770853957	20.4242000931
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C40	20.2547776269	-8.0887825857	19.1806475352
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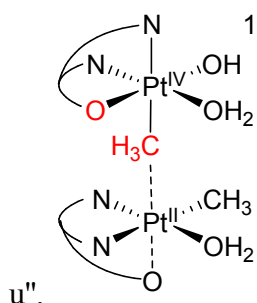
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H56	23.2847871350	-4.8641296886	20.8118504863
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H22	14.5622148042	2.1310709714	19.7586758369
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C36	19.7914148520	-3.6387855238	24.5622056312
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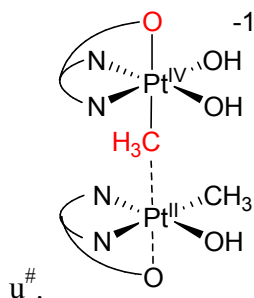
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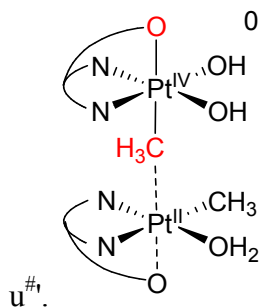
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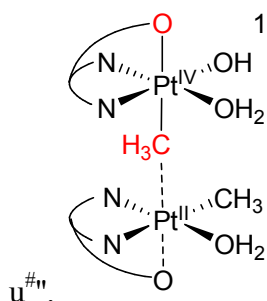
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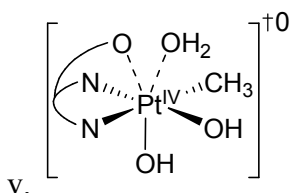
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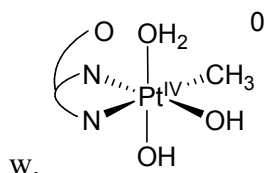
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C42	-4.5215824808	-4.0772029325	0.6752867405
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S46	-4.5249768290	-5.6844533383	-0.3118802006
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O48	-3.2619389915	-5.7044202908	-1.1378678614
O49	4.6344274980	2.1972803462	2.5850893905
O50	-4.5502163258	-6.7450881839	0.7272832519
O51	2.7257337412	2.9458722859	4.0331742162
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C54	-0.4181108289	-1.2597272747	-0.1643183176
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H59	-0.8000504126	-3.8409226556	-3.2297283347
H60	-0.5518944849	-0.8486268286	-1.1528644459
O61	0.0354755965	-4.5409269335	-0.8242478630
O62	1.3909047918	0.8666512630	-1.4176542601
H63	0.5642310037	-4.4075393314	-1.6340382748
H64	2.0321560830	1.5978523564	-1.4583051760
H65	-2.7866788266	-0.8772721305	-2.1149521808
H66	-1.7152237060	0.5716648534	2.0931403283
H67	2.4746950831	-1.1495489449	-1.1172784371
H68	-0.1658126058	-3.6917931161	1.9094912529
H71	-0.0251628451	1.4106120122	-2.3212002817
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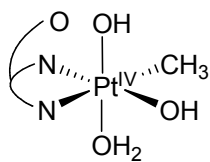


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C6	-2.0430244313	4.7284894026	5.7743980964
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C10	-1.9414350069	3.0972327332	9.1472391473
H11	-1.5602560751	4.5730405361	4.8201215298
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C13	1.4286804427	3.0107462784	10.8972351582
C14	2.2465328735	2.6315068694	9.8324858983
C15	1.6606105636	2.4109386433	8.5888199890
N16	0.3379506612	2.5363718674	8.3831378196
C17	-0.4597716475	2.9222749376	9.4005208537
C18	0.0597110882	3.1641792085	10.6755126375
H19	1.8490724957	3.1953318975	11.8829270731
H20	3.3197459915	2.5140522691	9.9516749359
H21	2.2629344443	2.1379551824	7.7266781124
H22	-0.6047553591	3.4764182746	11.4768603434
H23	-2.3786230673	3.5567343181	10.0376039005
S24	-2.8060920743	1.4340843102	9.1112307762
O25	-2.9214684854	1.0419109187	10.5398109384
O26	-4.1005517272	1.6546299757	8.4174142951
O27	-1.8558933096	0.5436389591	8.3535525121
C28	-1.1934786907	2.0941824110	4.3158565590
H29	-2.2826213623	2.1517284880	4.3605488554
H30	-0.7690285417	2.9277379045	3.7513280174
H31	-0.8700035556	1.1406069850	3.9011917656
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O39	-1.8325210276	-0.2697544403	5.8181472178
H40	-0.8609231039	-0.3750653187	5.7683281104
H42	-2.0205251722	-0.2832924791	6.7768589817
O40	2.0376499699	1.9525322456	3.6743427576
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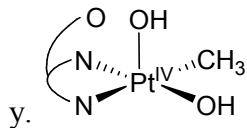
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C6	0.6885412192	-2.4451969366	-1.1513164727					
C7	0.8229541437	-3.7583079335	-1.5752602542					
H8	-0.2569177592	-5.6000133475	-1.9459355254					
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C10	-2.9814828126	-2.2281100044	-0.3363510648					
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H12	1.8004799664	-4.1199857370	-1.8810120874					
C13	-5.4259778627	0.4708950175	-1.3737729667					
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C17	-3.5161064142	-0.8729428891	-0.7448048884					
C18	-4.8843337667	-0.7660492530	-1.0312908906					
H19	-6.4867267745	0.5627431074	-1.5934042726					
H20	-4.9524698314	2.5684469368	-1.6974245114					
H21	-2.5299035601	2.2278020460	-1.1771188743					
H22	-5.5127742708	-1.6497267609	-0.9790678732					
H23	-3.6701787425	-2.9599930903	-0.7669910392					
S24	-3.3097034381	-2.5838375914	1.5032402605					
O25	-2.7907408784	-1.4069609366	2.2892076391					
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O27	-2.5772124735	-3.8423587929	1.7923111699					
C28	1.5407867560	0.2867428844	0.0759364056					
H29	2.1605707513	0.2518499286	-0.8254030560					
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H31	1.7622321846	-0.5549266264	0.7360670858					
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H36	-0.1871017109	2.5458808516	-1.0893203163					
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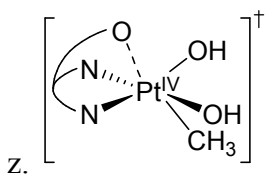
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C6	0.6128368799	-2.5214911264	-1.3550272754					
C7	0.7511160655	-3.8826409232	-1.5800418881					
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C15	-3.2663325906	1.3445065326	-1.1520312863					
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C17	-3.5118791164	-0.9392900533	-0.7875549243					
C18	-4.8445252338	-0.8806153250	-1.2174284449					
H19	-6.4181087111	0.3941913377	-1.9605914711					
H20	-4.9590640657	2.4531140590	-1.8728944134					
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H23	-3.6761848420	-3.0198611072	-0.6114895025					
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O25	-3.0378266315	-1.0242231757	2.2031965374					
O26	-4.7905929930	-2.6918870721	1.6566251504					
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C28	1.5780403169	0.1969685871	-0.1544312412					
H29	2.0784436561	0.2197631770	-1.1273570001					
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H35	-1.4341802814	-0.4484107756	1.7395615328					
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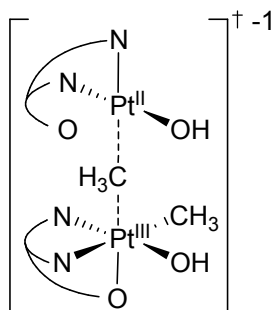
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H8	-0.2215066081	-5.7324326900	-1.4817133532					
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C17	-3.6115745228	-0.9128256921	-0.6020540372					
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O27	-2.6228046234	-1.1134451444	2.1887760581					
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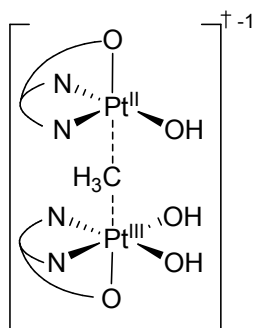
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S24	-2.8324821194	-2.2325084336	1.6638263903					
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O37	-1.0204695354	2.0964466583	-0.2629079572					
H38	-0.2521766888	2.4259777764	0.2507134027					
O39	1.2586523419	2.4908515865	1.4383551831					
H40	2.1226723143	2.5629232306	1.0066227258					
H41	1.0701627885	1.5254377841	1.4575505641					



methyl-transfer between Pt(II)-Pt(III), G=41.4 kcal/mol at pH=14

	-2938.58145	-2938.72993	-2939.29894	338.33	29.17	173.06	260.07	-1844230.8
Pt1	-1.3192978366	-1.7010955301	8.8174010386					
C2	-2.5352756710	2.4613768666	6.5676110865					
C3	-1.6945214382	1.5384662004	5.9575187528					
C4	-1.3602641672	0.3413833790	6.6021336196					
N5	-1.8548445192	0.0557750291	7.8375125057					
C6	-2.6790170780	0.9604906795	8.4260221291					
C7	-3.0366691780	2.1614374269	7.8331160083					
H8	-2.7910664670	3.3908342007	6.0674790836					
H9	-1.2814916246	1.7385767016	4.9744150241					
C10	-0.4082222992	-0.5871051827	5.8835556999					
H11	-3.0374060691	0.7170821960	9.4178020062					
H12	-3.6968908030	2.8409067951	8.3632233128					
C13	-0.8476331741	-4.0972291912	4.5202353023					
C14	-1.2704276827	-4.7645910780	5.6706348055					
C15	-1.4056048429	-4.0380624800	6.8452452314					
N16	-1.1352571866	-2.7169475935	6.9156234133					
C17	-0.7321245480	-2.0571584785	5.8110449898					
C18	-0.5813303495	-2.7331663077	4.5938454193					
H19	-0.7305928065	-4.6301446798	3.5807069892					
H20	-1.4966053959	-5.8262295614	5.6655463272					
H21	-1.7290618877	-4.5042985938	7.7691397467					
H22	-0.2515656371	-2.1852250977	3.7171290777					
H23	-0.3721021876	-0.2350779423	4.8510236128					
S24	1.3911569487	-0.2908982139	6.3620389941					
O25	1.6065356300	-0.7557924554	7.7605740820					
O26	2.1359929084	-1.0997228727	5.3605882467					
O27	1.5495062906	1.1784416714	6.2031150597					
H28	-4.4939996110	1.5990487120	14.9404516565					
O29	-4.9872453793	1.7343811194	14.1155059883					
H30	-4.3244327144	1.5849398544	13.4005290821					
O31	-0.6162547732	-3.3293794033	9.8469771970					
H32	-0.1382591341	-3.8856593666	9.2147828420					
H33	-2.4253059728	-0.5552742559	10.8441617054					
C34	-1.4139092504	-0.7628600865	11.1674233060					
H35	-0.5895902382	-0.2294618080	10.7087236562					
H36	-1.2000025012	-1.7546970024	11.5469917817					
Pt101	-1.6371162037	0.4583513305	13.0266245726					

C102	1.9541592365	-1.4623055631	15.7264562184
C103	0.6934671235	-1.2251272358	16.2695331753
C104	-0.3356090979	-0.7453755660	15.4587638478
N105	-0.1178907220	-0.4808910013	14.1438176761
C106	1.0876490761	-0.7576464777	13.6042904018
C107	2.1453160621	-1.2440748888	14.3644098534
H108	2.7622849642	-1.8269041012	16.3545116648
H109	0.4958979162	-1.4137356275	17.3199453480
C110	-1.7091417141	-0.5461513905	16.0571941179
H111	1.1947294638	-0.6135332017	12.5348600221
H112	3.0974937050	-1.4427524224	13.8831844861
C113	-4.7876304613	-2.6532438563	15.3575584766
C114	-4.9869542958	-2.3463286865	14.0117575644
C115	-4.0911481493	-1.4868264304	13.3851732091
N116	-3.0388709624	-0.9533602885	14.0273824210
C117	-2.8478540883	-1.2273557947	15.3328063104
C118	-3.7074447850	-2.0813349006	16.0268675883
H119	-5.4667298397	-3.3190866964	15.8829971980
H120	-5.8215754651	-2.7569486721	13.4522628721
H121	-4.2145834230	-1.2012697813	12.3462811769
H122	-3.5320282062	-2.2837387975	17.0790111387
H123	-1.6848255201	-0.9325914799	17.0780245868
S124	-2.0852457817	1.2598443973	16.3321621130
O125	-1.7555457801	1.9548163218	15.0405408240
O126	-3.5415791120	1.3092507478	16.6443771013
O127	-1.1995102227	1.6705332067	17.4473074571
H128	0.8417138672	-2.3873945457	10.3624642004
O129	1.6191950972	-1.7888632582	10.4607066816
H130	1.6133500748	-1.3265198632	9.6062666450
O131	-3.2202533213	1.3291914529	12.0753753528
H132	-2.9390775170	2.2109352256	11.7889261689
H133	-0.3254418730	2.7166413147	12.9296267492
C134	-0.3793253239	1.8846180287	12.2204420440
H135	-0.7762323038	2.2432771542	11.2649023153
H136	0.6259507329	1.4857368825	12.0574266757

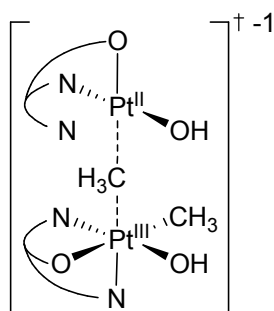


methyl-transfer between Pt(II)-Pt(III), G=52.5 at pH=14

-2938.56521	-2938.73687	-2939.28910	339.49	29.05	171.19	258.16	-1844237.6
Pt1	15.5992658329	-2.3072801858	18.8916672968				

C2	11.6921617302	-2.7065338937	21.7697117162
C3	11.5506271895	-2.6811202041	20.3863533804
C4	12.6720637642	-2.5436578161	19.5623810116
N5	13.9141482027	-2.4370716085	20.1009132971
C6	14.0481951485	-2.4604370682	21.4458556691
C7	12.9717003595	-2.5899585614	22.3097687828
H8	10.8220964676	-2.8142350263	22.4107884293
H9	10.5698816032	-2.7658413466	19.9300647851
C10	12.4652990304	-2.4853069221	18.0698435150
H11	15.0567765018	-2.3702159311	21.8256522624
H12	13.1443014542	-2.6003710918	23.3812020155
C13	13.2983796558	-4.9532679873	15.3228669867
C14	14.6515294247	-5.1664660295	15.5815291334
C15	15.2393143015	-4.5078794741	16.6558198145
N16	14.5553352302	-3.6631360876	17.4532255100
C17	13.2419100305	-3.4577739947	17.2154960310
C18	12.5871489601	-4.0953977359	16.1567454805
H19	12.8039948512	-5.4430665526	14.4882497010
H20	15.2524840066	-5.8257891550	14.9623490848
H21	16.2928566296	-4.6381908935	16.8767342267
H22	11.5326203411	-3.9038564845	15.9870449710
H23	11.4057543015	-2.6778362397	17.8900088740
S24	12.6197729710	-0.7317001836	17.4275223244
O25	14.0407331650	-0.3179240866	17.6296149487
O26	12.2324724140	-0.8393040541	15.9964371123
O27	11.6608320099	0.0360867443	18.2658906918
C28	16.4566475469	-0.7652324979	19.9588195937
H29	15.8948579695	-0.5300042584	20.8691241393
H30	17.4966671022	-0.9742057073	20.2346167032
H31	16.4376190359	0.1194892061	19.3121704650
O32	17.1986823136	-2.2544273572	17.6361976703
H33	17.8280920658	-1.6080091774	17.9863545838
Pt34	18.9714284461	-5.0004326420	21.2568017516
C35	18.2208445153	-2.8119966638	25.5439574895
C36	19.2952744872	-2.4026780951	24.7644288210
C37	19.5567719170	-3.0056314715	23.5266913326
N38	18.7563730826	-4.0033530022	23.0688763090
C39	17.6950441449	-4.3850282762	23.8246554822
C40	17.3967861322	-3.8264758397	25.0562217299
H41	18.0244750090	-2.3401324021	26.5021153855
H42	19.9488499088	-1.6067822455	25.1063665526
C43	20.7631379183	-2.5049768893	22.7687987189
H44	17.0833303125	-5.1757993938	23.4061388136
H45	16.5365434271	-4.1865854608	25.6110189027
C46	21.2040356340	-0.6612565030	19.4986702710
C47	20.7550572063	-1.6382359040	18.6117945023

C48	20.2489874285	-2.8301904494	19.1269875708
N49	20.1802229785	-3.0815391046	20.4458830205
C50	20.6510087918	-2.1616862849	21.3076648394
C51	21.1578415382	-0.9332852202	20.8632173829
H52	21.5957187885	0.2864635254	19.1378015308
H53	20.7935753937	-1.4886896633	17.5365709598
H54	19.8927630543	-3.6061061321	18.4619223466
H55	21.5229328604	-0.2093871758	21.5849707483
H56	21.0793345339	-1.5967730131	23.2846447662
S57	22.2910240274	-3.5722059549	23.0086852044
O58	22.2237156514	-4.6845327514	22.0130199510
O59	23.4044536844	-2.6258056545	22.7393524185
O60	22.2050541124	-4.0424361258	24.4155435684
C61	17.0444009502	-3.8020889272	20.2525643504
H62	17.6517072484	-3.7952991959	19.3692071615
H63	16.3100015956	-4.5838355153	20.3978810354
H64	17.1598183357	-3.0373456770	21.0007422651
O67	19.1359109610	-5.9797709854	19.4582668709
H68	18.7446946729	-6.8612347744	19.5500929231
O69	18.5001040907	-4.6226182011	17.0707964146
H70	18.0702422072	-3.7645320001	17.2969795216
H71	18.5788064384	-5.1439847251	17.9007022075
O78	21.8265228792	-5.5941755088	19.2878311191
H79	21.9507231362	-5.1252801003	20.1288862778
H80	20.8636931534	-5.7980835517	19.2919293545

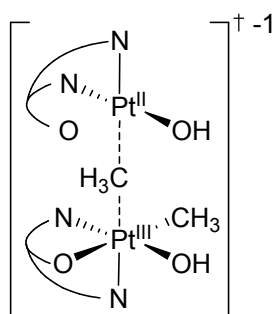


methyl-transfer between Pt(II)-Pt(III), G=59.7 at pH=14

	-2938.54532	-2938.71996	-2939.27084	338.15	28.61	173.19	260.20	-1844230.4
Pt1	15.0802023797	-1.9561395883	19.3358836441					
C2	12.2166295841	-0.0692628224	15.5418891964					
C3	11.9002160058	-1.2745858273	16.1686120661					
C4	12.6855510571	-1.7056277126	17.2414481431					
N5	13.7233221840	-0.9766309193	17.6801009592					
C6	14.0363710754	0.1794124063	17.0799245911					
C7	13.3065974115	0.6717700519	16.0008962316					
H8	11.6247713014	0.2806732470	14.7003237598					
H9	11.0660667151	-1.8796913468	15.8271636105					
C10	12.4410994312	-3.0462631812	17.8997744673					
H11	14.9072350490	0.6976219717	17.4682618576					

H12	13.5948270534	1.6082122001	15.5328971805
C13	10.9314819633	-3.5650528302	21.3411241122
C14	11.9983030516	-3.1762435458	22.1492567043
C15	13.1692872671	-2.7393054947	21.5452473581
N16	13.3127395182	-2.6783165255	20.2047018409
C17	12.2837902956	-3.0587260770	19.4047101160
C18	11.0828738298	-3.5061472586	19.9583155752
H19	9.9994344706	-3.9142396431	21.7763204633
H20	11.9376732699	-3.2107342406	23.2321110789
H21	14.0232582311	-2.4319779555	22.1352596679
H22	10.2771404812	-3.8094656648	19.2977080235
H23	11.5336812829	-3.4757655557	17.4697134918
S24	13.7425849070	-4.2722599833	17.3749531191
O25	15.0563235812	-3.7697747720	17.9450925795
O26	13.3171847984	-5.5574080616	17.9702748832
O27	13.7356945757	-4.2274803455	15.8932905989
C28	15.0707860355	-0.2903981732	20.5424319519
H29	14.0523116846	0.1069227169	20.5660556848
H30	15.3945367460	-0.5327854239	21.5581115761
H31	15.7436369658	0.4601515096	20.1161186577
O32	16.7044439989	-1.2434259002	18.3475643698
H33	17.1527910378	-0.5873514643	18.9008403665
Pt34	18.6595403718	-4.2123082709	21.2076776590
C35	18.9906219019	-8.3147283540	25.6731744679
C36	19.8238265447	-7.2600652459	25.3080899544
C37	19.3328810929	-6.2650793804	24.4497577996
N38	18.0800535356	-6.2859054669	23.9728303811
C39	17.2814117761	-7.3015096879	24.3418792584
C40	17.6864114296	-8.3390274138	25.1797520983
H41	19.3522371507	-9.0977127617	26.3345820090
H42	20.8433397432	-7.2062294874	25.6776832425
C43	20.2815116970	-5.1379828897	24.0600311512
H44	16.2690864816	-7.2856410108	23.9429116069
H45	16.9950606425	-9.1363772524	25.4366750384
C46	19.6556491019	-1.5896737797	25.2075111232
C47	19.0409638407	-1.0366128982	24.0863999830
C48	18.8013145271	-1.8518465344	22.9923201081
N49	19.1275671287	-3.1695814636	22.9463763791
C50	19.7596337528	-3.7093463887	24.0256247031
C51	20.0210866877	-2.9302818622	25.1589388526
H52	19.8649683305	-0.9899509246	26.0884149451
H53	18.7553878233	0.0096633861	24.0433273247
H54	18.3435811962	-1.4509083588	22.0976549460
H55	20.5279894600	-3.3903116045	26.0016199428
H56	21.0636923037	-5.1315402813	24.8243013588
S57	21.3163009320	-5.5743202107	22.5926713134

O58	20.3870202427	-5.6918350706	21.3980361226
O59	22.2766099683	-4.4519854005	22.4560610538
O60	21.9247432164	-6.8854615555	22.9153988864
C61	16.5710847549	-3.1207716485	20.7116430618
H62	17.3066898025	-2.7176188813	20.0258834530
H63	16.1300941068	-4.0952114357	20.5417693723
H64	16.4078514282	-2.6505347191	21.6730503938
O67	18.1788121045	-5.2642936434	19.5091315648
H68	18.9260135006	-5.8600052801	19.3439469688
O69	18.2822290052	-3.3666472659	17.5718310967
H70	17.6851697067	-2.6383599566	17.8440295735
H71	18.1526326784	-4.0713554816	18.2512559215
O78	16.4713886792	-6.6188128618	21.1549681793
H79	16.9183437116	-6.2228946346	21.9196113733
H80	17.0064479468	-6.2440998058	20.4146682881

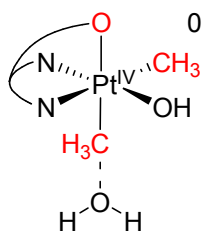


methyl-transfer between Pt(II)-Pt(III), G=48.7 at pH=14

	-2938.55338	-2938.73566	-2939.28254	338.81	28.36	170.76	257.74	-1844241.4
Pt1	15.2078307504	-1.9343929836	19.4754993666					
C2	12.1608111042	0.1095366237	15.8601378021					
C3	11.9011027349	-1.1484464538	16.4037486730					
C4	12.7462575640	-1.6364738469	17.4043699427					
N5	13.7873155685	-0.9194275482	17.8487250313					
C6	14.0464008298	0.2867505593	17.3275758069					
C7	13.2545546364	0.8418992637	16.3254890205					
H8	11.5219239955	0.5080355796	15.0766355841					
H9	11.0664977456	-1.7479437023	16.0531566031					
C10	12.5613868649	-3.0249088055	17.9775136091					
H11	14.9242801218	0.7925659383	17.7173543416					
H12	13.4971262433	1.8193057409	15.9197191871					
C13	11.1008567762	-3.7824756776	21.3939811652					
C14	12.1553616766	-3.3935344086	22.2174347171					
C15	13.3097107601	-2.8909840785	21.6315431583					
N16	13.4517919762	-2.7609869477	20.2962823140					
C17	12.4301029894	-3.1343122569	19.4817370424					
C18	11.2481856143	-3.6522165802	20.0158471466					
H19	10.1815428815	-4.1827559963	21.8121722344					
H20	12.0979765009	-3.4773649995	23.2978651833					
H21	14.1552737206	-2.5842733089	22.2342952548					

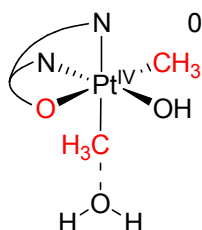
H22	10.4509453600	-3.9507276227	19.3427835543
H23	11.6600382848	-3.4576782227	17.5377284592
S24	13.8861447015	-4.1660838992	17.3480994054
O25	15.1786223366	-3.7373509130	18.0123597180
O26	13.4436718164	-5.5158267534	17.7672085495
O27	13.9101327658	-3.9521087361	15.8802298350
C28	15.1030067233	-0.3035613969	20.7181005966
H29	14.0706922368	0.0579978306	20.7089675571
H30	15.3959592519	-0.5624022078	21.7388522123
H31	15.7656273366	0.4776365028	20.3331325363
O32	16.7859913358	-1.0985448859	18.5010814234
H33	17.2639744258	-0.5178542444	19.1108135129
Pt34	18.9786704170	-4.0563969591	21.3177963860
C35	20.6189994632	-1.5621732651	25.1786336231
C36	20.5744089222	-2.9514606847	25.1953456750
C37	20.0797963667	-3.6569818092	24.0931332118
N38	19.6000502714	-3.0043790630	23.0008897911
C39	19.6450923178	-1.6490632180	22.9912187263
C40	20.1522162700	-0.8990547536	24.0436922210
H41	21.0219787245	-1.0132009572	26.0252066278
H42	20.9386965285	-3.5065645588	26.0540701037
C43	20.1479475901	-5.1631931026	24.1277219457
H44	19.2720871021	-1.1717981792	22.0931974062
H45	20.1857293026	0.1828889446	23.9637438790
C46	22.5793586043	-7.3422487146	22.2032263526
C47	22.2913465562	-6.9504721257	20.8947565058
C48	21.3054519667	-5.9944142728	20.6913670148
N49	20.6161291597	-5.4373516045	21.7089549515
C50	20.8819301562	-5.8096965402	22.9773298318
C51	21.8666841618	-6.7656685292	23.2499952605
H52	23.3531523049	-8.0771594663	22.4064137432
H53	22.8233386925	-7.3645244605	20.0444554415
H54	21.0551224878	-5.6431772412	19.6957876122
H55	22.0713006581	-7.0423336142	24.2796183944
H56	20.7139540040	-5.4206123357	25.0244607829
S57	18.5202340435	-5.9838669752	24.5788603743
O58	17.4373086252	-5.4758665019	23.6871758612
O59	18.7994119711	-7.4332897226	24.4120218038
O60	18.3352640214	-5.5536602972	25.9921831652
C61	16.8070223081	-2.9558689855	20.8387200323
H62	17.5476950041	-2.5791524325	20.1425649049
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O67	18.3302081842	-5.0796594072	19.6532863291
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O69	18.3520390771	-3.2122550558	17.6652998063

H70	17.7600631593	-2.4840126574	17.9527305783
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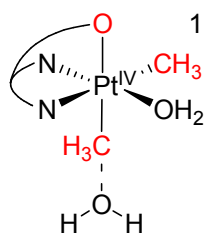
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H8	-1.1664014072	-5.9377163052	-0.1390122885					
H9	-2.9646853874	-4.4184851764	0.6894311075					
C10	-2.9336834089	-1.7330746608	0.8059652316					
H11	1.1783268253	-2.4273075790	-1.0109481500					
H12	0.9573796319	-4.9107471819	-1.0301181261					
C13	-5.0839842948	0.8332202730	-0.9538870321					
C14	-4.1104955901	1.6992368492	-1.4489040352					
C15	-2.7771907067	1.4241638232	-1.1851603914					
N16	-2.3722918798	0.3547375700	-0.4607633426					
C17	-3.3113860864	-0.5131435652	0.0010065595					
C18	-4.6713615932	-0.2824566171	-0.2340409617					
H19	-6.1404552982	1.0168891270	-1.1271950199					
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H21	-1.9991049549	2.0787703727	-1.5519600762					
H22	-5.3990294177	-0.9842011102	0.1599669607					
H23	-3.8345630902	-2.3458516069	0.8761287316					
S24	-2.6724877726	-1.3169569787	2.6153577758					
O25	-3.9444867626	-0.6495418266	3.0039665659					
O26	-2.4610310640	-2.6435054284	3.2547686863					
O27	-1.4873516238	-0.4182120337	2.7002722996					
C28	0.4768747542	0.6544729376	-2.5068247546					
H29	0.5579697732	1.6575283531	-2.1201312086					
H30	1.2689703447	-0.0532158108	-2.3058613993					
H31	-0.4858176663	0.2806175664	-2.8240832197					
H33	1.0331576046	2.2886215459	0.4939094604					
O34	1.5689497540	-0.2892922067	0.5139988839					

O37	1.0541111289	1.0473392800	-4.2186084079
H38	0.5198876178	1.7858980197	-4.5665933554
H39	1.9477296820	0.5416887563	0.8354110694
H47	1.9611072442	1.4022249046	-4.1633195555
O48	3.1310909857	-1.1063920042	-1.4530594117
H50	2.5862000148	-0.7911547906	-0.6783457080
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C41	-0.0386963490	2.0813175248	0.3723401138
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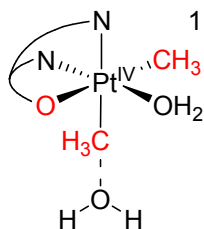
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N5	-0.2086409175	-1.8707111323	-0.5911101179					
C6	-0.5898848967	-2.3422149389	-1.8013924855					
C7	-0.5965648473	-3.6914417526	-2.1251555673					
H8	-0.1923639554	-5.6778548434	-1.3682650859					
H9	0.5952756785	-4.8121851674	0.8357977522					
C10	0.8363687713	-2.3011875133	1.6547973424					
H11	-0.9039657908	-1.6036586342	-2.5263002494					
H12	-0.9158057468	-3.9979327015	-3.1164491485					
C13	-0.5013794665	-1.5057244265	5.1153430537					
C14	-1.7409039201	-0.9615078666	4.7762794730					
C15	-2.0860617642	-0.8987808632	3.4270349580					
N16	-1.2837847694	-1.3220084813	2.4371208081					
C17	-0.0939017744	-1.8408313805	2.7678425794					
C18	0.3339000392	-1.9603288345	4.0969150732					
H19	-0.1915502816	-1.5814099628	6.1541789627					
H20	-2.4306230117	-0.6019805370	5.5344731576					
H21	-3.0517470087	-0.4978874187	3.1248688621					
H22	1.3036319015	-2.3923092557	4.3222793228					
H23	1.4179680331	-3.1439353809	2.0390456317					
S24	2.1634415415	-1.0440579666	1.3619902070					
O25	2.9656886584	-0.9875173306	2.6044816010					
O26	2.9019188148	-1.4969301495	0.1577175086					
O27	1.4230001762	0.2635422114	1.1316305619					
C28	1.4206174982	0.8182551121	-1.9701169715					

H29	1.5664104985	1.6850918777	-1.3352382931
H30	1.8370710010	-0.1309863887	-1.6666026465
H31	0.6582247125	0.8492315354	-2.7357199732
O32	-0.7195391217	2.1408885529	0.2304888581
H33	-1.2591609790	2.1499453543	1.0349563427
O35	2.7953284858	1.2695311824	-3.1551344729
H36	3.0048550679	0.4904992397	-3.7026882706
H37	-2.7273652336	1.1167308095	-0.9882571907
H43	3.6107784836	1.4506265409	-2.6527496876
O48	1.7574832210	3.0051454860	0.5378536563
H49	2.0985657984	2.1732771844	0.9009273534
H50	0.7887294510	2.7793201256	0.4708152756
C41	-2.1310991291	0.2677175508	-1.3382808461
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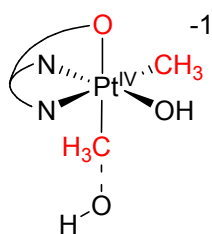
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N5	-0.8521838230	-2.2143497348	-0.2532863920					
C6	0.0430637824	-3.0946361938	-0.7398765664					
C7	-0.1226697213	-4.4689038902	-0.6183480284					
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C10	-2.9326859036	-1.6683834354	0.9386095302					
H11	0.9184845390	-2.6711936479	-1.2176074914					
H12	0.6302004764	-5.1398933306	-1.0195753984					
C13	-5.1028593631	0.7768705422	-0.9689668089					
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C15	-2.7993670475	1.3537619608	-1.2657774104					
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C17	-3.3237427844	-0.5070810347	0.0572481666					
C18	-4.6840398972	-0.2839016709	-0.1730357553					
H19	-6.1609730034	0.9439677128	-1.1484857072					
H20	-4.3996342572	2.4548412658	-2.1564825009					
H21	-2.0279218607	1.9876188413	-1.6788961231					
H22	-5.4084373635	-0.9541658615	0.2778710058					
H23	-3.8532558951	-2.2047538790	1.1749843189					

S24	-2.3895610750	-1.1221615640	2.6514438575
O25	-3.3994770381	-0.1060113410	3.0445319757
O26	-2.4390402550	-2.3799165665	3.4416900049
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C28	0.2449644801	0.5359383125	-2.6560193645
H29	0.3651809600	1.5360978309	-2.2722163670
H30	1.0466035499	-0.1792087992	-2.5380357642
H31	-0.7354458239	0.1676724576	-2.9209768678
H33	1.0948648299	2.0742291506	0.2907119445
O34	1.5546898217	-0.6439869425	0.3420225300
O37	0.7059549347	0.9601327615	-4.4143221030
H38	0.0758872133	1.6223270880	-4.7564419273
H39	1.5652478672	-0.9180159416	1.2745995137
H47	1.5649184099	1.4228127289	-4.4038385631
H50	2.3799867507	-0.0786334317	0.2068808873
H51	4.3600012871	0.0558703301	-0.6261584622
C41	0.0097684674	1.9343786442	0.2373458776
H42	-0.3947715983	2.6232964858	-0.5120339494
H43	-0.4281211794	2.1883422465	1.2093806777
O43	3.8505883275	0.5639842111	0.0259906775
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C3	0.4109889812	-4.0571693718	0.0263018373					
C4	0.3301953770	-2.6946676109	0.3223634594					
N5	-0.2148487509	-1.8258440041	-0.5747668728					
C6	-0.6404958907	-2.3047731649	-1.7688636537					
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H9	0.8492766278	-4.7259145115	0.7598579758					
C10	0.9032958915	-2.2302995750	1.6442421196					
H11	-1.0451571540	-1.5843570597	-2.4652581861					
H12	-0.9344216135	-3.9605482939	-3.0865517643					
C13	-0.7398912708	-1.8327107250	5.0405132303					
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C15	-2.0719224086	-0.8338075279	3.3171472730					
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C17	-0.0880597358	-1.8368956532	2.7272218704					

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H20	-2.6433136986	-0.8542817831	5.3961595576
H21	-2.9628110975	-0.3037077144	2.9870076062
H22	1.0812556676	-2.7399765278	4.3049555157
H23	1.5025740876	-3.0592451896	2.0299107325
S24	2.2046528805	-0.9400998470	1.3981050790
O25	2.9349798219	-0.8315488327	2.6761717565
O26	3.0028200168	-1.3849616196	0.2310772977
O27	1.4411094793	0.3492787113	1.0974021829
C28	1.3304265272	0.6213320445	-2.0784132662
H29	1.3865197390	1.6348656563	-1.7080420711
H30	1.8640167467	-0.1633865733	-1.5628060421
H31	0.5764968845	0.3858866951	-2.8150651369
O32	-0.6882681344	2.2363940419	0.2266451718
H33	-1.2688558728	2.3752842722	0.9938091009
O35	2.6620329170	0.8984194464	-3.3910424964
H36	2.9001241412	0.0372296607	-3.7821291969
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H43	3.4804324745	1.2122911951	-2.9639107847
H49	2.0799890672	2.1908455730	0.9339261041
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C41	-2.1792130357	0.2721846348	-1.2317170973
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C4	-1.1504948537	-2.8044221837	0.4419570516					
N5	-0.1840204805	-1.9291683695	0.0988788504					
C6	1.0962554410	-2.3448329525	0.0577885262					
C7	1.4719607356	-3.6444088378	0.3754928601					
H8	0.7327371476	-5.5793560371	1.0032964949					
H9	-1.6427720198	-4.8107906594	1.0436214367					
C10	-2.5817964025	-2.3356809942	0.5370286963					
H11	1.8289995728	-1.5949553761	-0.2152402133					

H12	2.5197378524	-3.9264597372	0.3417312663
C13	-4.8347871211	-1.0843343353	-2.2375644452
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N16	-2.5088642466	-0.2979499033	-0.9018484892
C17	-3.1176130199	-1.4658808038	-0.5724361938
C18	-4.2805491465	-1.8730330640	-1.2346570751
H19	-5.7321572023	-1.4046647615	-2.7588588125
H20	-4.5933634966	0.7840635039	-3.3234191199
H21	-2.5465886435	1.3950684709	-2.1012226989
H22	-4.7410354957	-2.8153081887	-0.9571336105
H23	-3.2098025074	-3.2280498366	0.5693079870
S24	-2.9359111926	-1.5860529223	2.2159850474
O25	-4.3986470714	-1.3191710147	2.1836575357
O26	-2.5299316590	-2.6506660695	3.1709484222
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H31	-0.5511867813	-0.3152518806	-2.6860391994
H33	-0.1366089176	2.8135080078	0.1195079667
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H36	-0.2339635227	1.4018928731	-4.4865670201
O37	0.5522469049	0.8651938186	-4.3055577387
H38	1.1360887424	0.9471509011	-5.8353691802
H39	1.1609966574	1.5392130832	1.0243771432
O40	1.4684166944	1.1420369239	-6.7624162044
H41	0.8297153923	1.7794205929	-7.1138599080
O43	3.4418429921	2.8522371115	-5.7211811461
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H45	2.8005758853	2.2686225516	-6.1763370777
O46	2.3074387002	2.5351299479	-3.2390771778
H47	1.6236728724	1.9429744185	-3.6733700715
H48	2.7297300656	1.9529717613	-2.5758236962
O47	3.1667008779	0.9024575995	-1.0904396114
H49	2.4442108058	0.7781167301	-0.4148608607
H50	3.6937465649	0.0916677523	-1.0801518694
C49	-1.0688930553	2.2447106035	0.0163332268
H51	-1.5953923026	2.6330576462	-0.8619632276
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